A simulation tool to model ozone retrieval uncertainties of Brewer and Dobson instruments

Luca Egli

Julian Gröbner, Ulf Köhler, Alberto Redondas, Virgilio Carreño and Henri Diemoz
("UVNews-Team")

and

Mario Blumthaler, Omar El Gawhary, Petri Kärhä, Ingo Kröger and Mark Weber
("ATMOZ Uncertainty Team")

EMRP
European Metrology Research Programme
Programme of EURAMET
The EMRP is jointly funded by the EMRP participating countries within EURAMET and the European Union

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EURAMET

Project ATMOZ

Main objective:
A traceable and harmonized global total column ozone network within 1%

5 Workpackages (WP):

- **WP 1:** Radiometric characterization of Dobson, Brewer & Array spectrordiometers
- **WP 2:** Development of array-based solar UV spectroradiometers
- **WP 3:**
  - Improved and consistent **ozone absorption cross-sections**
  - Validation of high resolution **extraterrestrial solar reference spectra**
  - **Comprehensive uncertainty budget** incorporating instrumental and atmospheric uncertainties
- **WP 4:** Creating Impact /Dissemination (Publications, Workshops, Campaigns, Training Commercialization)
- **WP 5:** Management (PMOD/WRC)

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Comprehensive Uncertainty Budget

Radiometry

Atmospheric Model

Measurement → **Total Column Retrieval Method** → **O_3 Value**

Uncertainty of **measurement:** + Uncertainty of **model:** = Uncertainty of **O_3 value**

Direct sun **measurement:**

- 4 Wavelengths: (Dobson/Brewer)
- Full spectrum: Array spectroradiometer

Beer-Lambert Law

$$I_\lambda = I_\lambda^0 e^{-\tau_\lambda m}$$

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Comprehensive Uncertainty Budget

Radiometry

Atmospheric Model

Measurement → **Total Column Retrieval Method** → **O_3 Value**

Uncertainty of **measurement:** +

- noise of the measurement
- wavelength uncertainty
- uncertainty of calibration
- bandpass uncertainty
- temperature gradients
- dead-time effect /linearity
- ND filter

Uncertainty of **model**:

- selected wavelengths (Brewer/Dobsons)
- selected cross-section
- selected atmospheric temperature
- extraterrestrial spectrum
- airmass uncertainty (atmospheric profile)
- rayleigh airmass uncertainty
- AOD /SO_2

= Uncertainty of **O_3 value**

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Sensitivity on Parameters

Sensitivity Analysis:

- Investigate **single contributions to overall uncertainty** budget
- Find the **most important parameter affecting** the overall budget
- Potential for **improvement** of measurement and/or retrieval.
- Calculate the **overall uncertainty budget**.

A software tool is needed for simulation the effect on different parameters

Uncertainty of **measurement:** + Uncertainty of **model**: = Uncertainty of **O_3 value**

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Uncertainty of **O_3 value**

Dependencies between measurement uncertainties and model uncertainties

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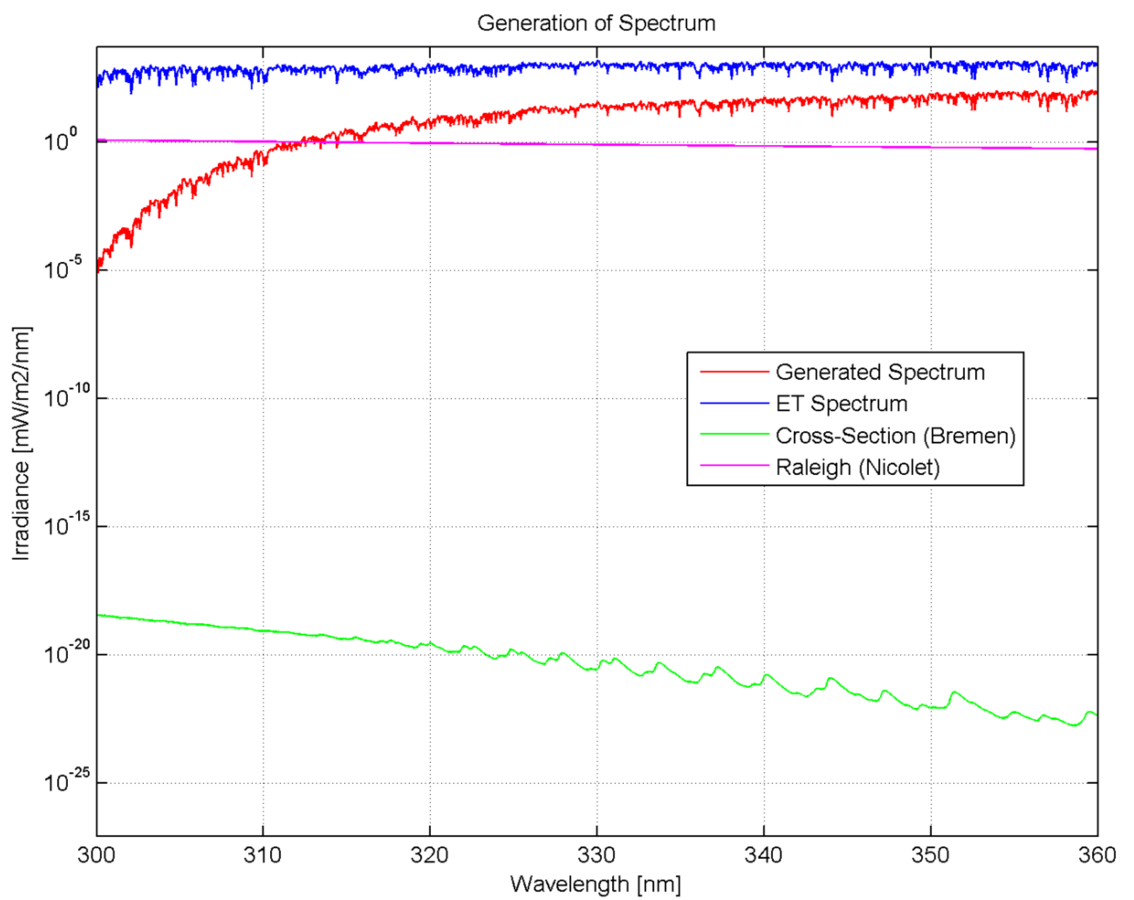
Procedure of Simulation

1. Generating spectrum (PMOD-model) between **300 – 360 nm** with **known parameters** and 49 atmosperic conditions 7 ozone x 7 airmass $I_\lambda = I_\lambda^0 e^{-\tau_\lambda m}$



FWHM as small as possible (=0.01 nm, ET)!

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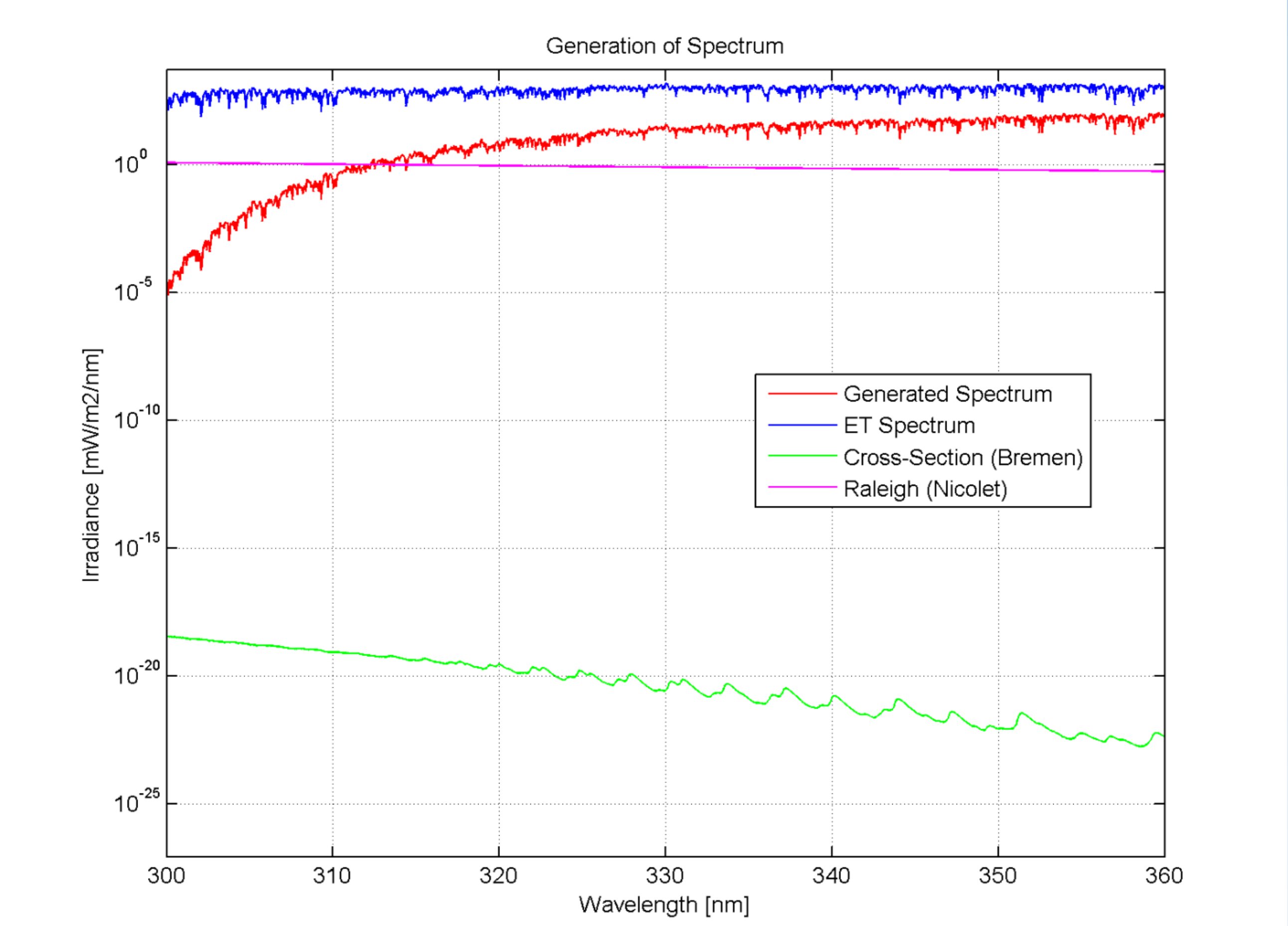


FWHM as small as possible (=0.01 nm, ET)!

Procedure of Simulation

2. Define retrieval method : **Double ratio technique** (Dobsons and Brewers)

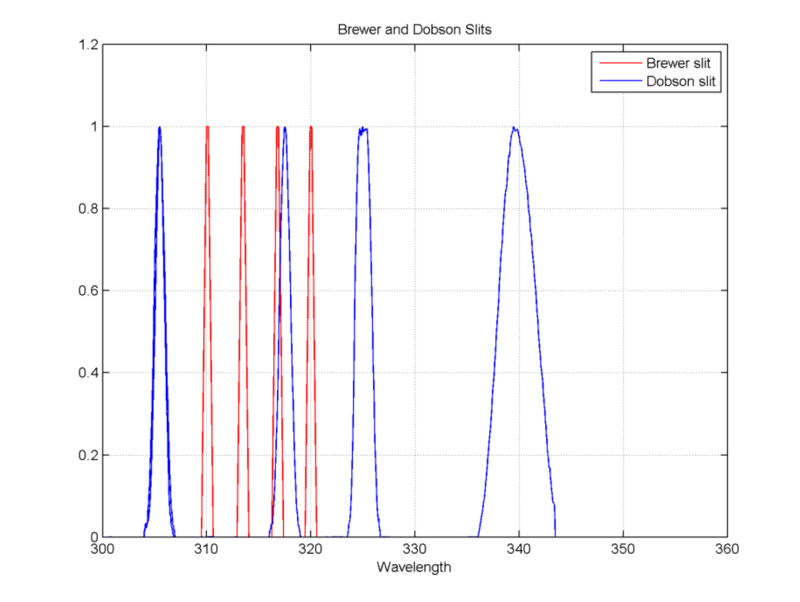
$$I_\lambda = I_\lambda^0 \mathrm{e}^{-\tau_\lambda m}$$ Beer-Lambert Law

$$\log I_i = \log I_i^0 - \tau_i^{\mathrm{R}} m_{\mathrm{R}} - \alpha_i^{\mathrm{O_3}} X m_{\mathrm{O_3}} - \tau_i^{\mathrm{aod}} m_{\mathrm{aod}}$$

m_{R}, $m_{\mathrm{O_3}}$, and m_{aod} are different airmasses due to different respective heights of the ozone, air and particle molecules within the different atmospheric profiles.

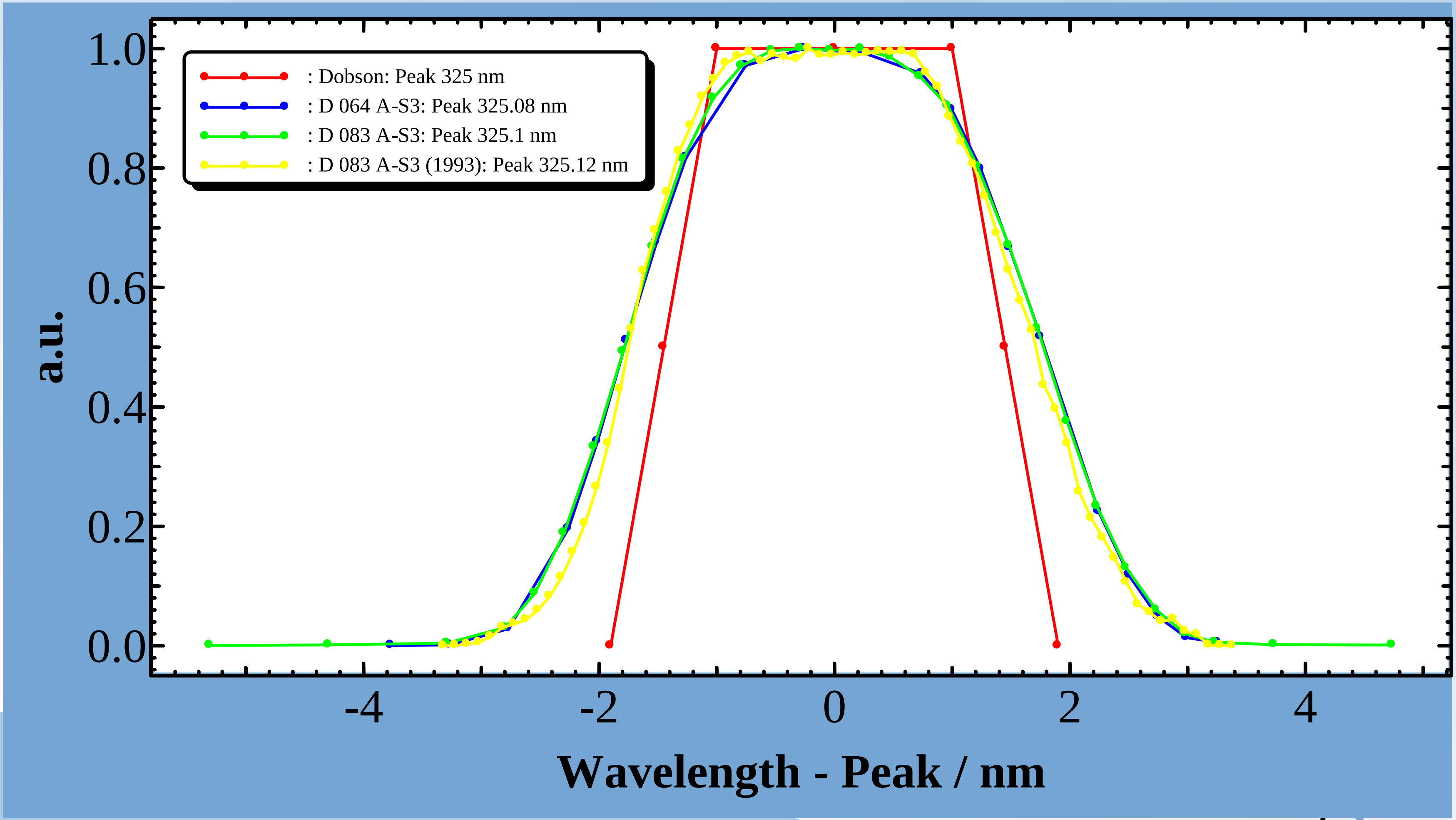
I_i^0= Extraterrestrial Spectrum, *i* = wavelength-index

i (slit)	**1**	**2**	**3**	**4**
λ-Brewer (nm)	310.1	313.5	316.8	320
λ-Dobson (nm)	305.51	317.62	325.08	339.97



Dobson Slits - D064

Dobsons D064 (DWD) and D083 (NOAA) characterized for wavelength and bandpass at PTB Braunschweig with tuneable laser facilities (Saulius Nevas)



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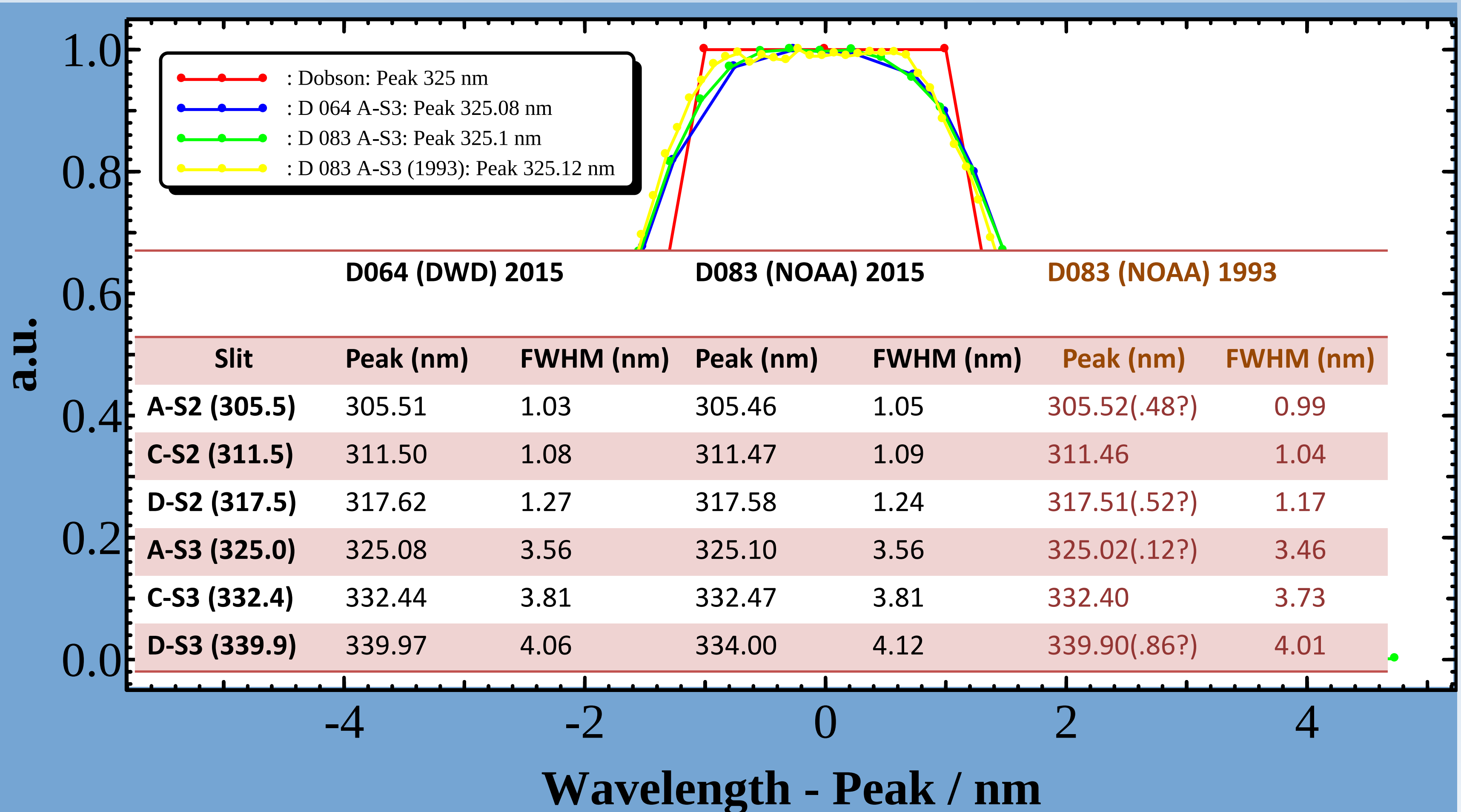

	D064 (DWD) 2015		D083 (NOAA) 2015		D083 (NOAA) 1993	
Slit	**Peak (nm)**	**FWHM (nm)**	**Peak (nm)**	**FWHM (nm)**	**Peak (nm)**	**FWHM (nm)**
A-S2 (305.5)	305.51	1.03	305.46	1.05	305.52(.48?)	0.99
C-S2 (311.5)	311.50	1.08	311.47	1.09	311.46	1.04
D-S2 (317.5)	317.62	1.27	317.58	1.24	317.51(.52?)	1.17
A-S3 (325.0)	325.08	3.56	325.10	3.56	325.02(.12?)	3.46
C-S3 (332.4)	332.44	3.81	332.47	3.81	332.40	3.73
D-S3 (339.9)	339.97	4.06	334.00	4.12	339.90(.86?)	4.01

Procedure of Simulation

«Double ratio» /«weighted ratio» technique (Dobsons and Brewers): combining all four wavelengths

$$F = F_0 - \Delta\tau^{\mathrm{R}} m_{\mathrm{R}} - \Delta\alpha^{\mathrm{O_3}} X m_{\mathrm{O_3}} - \Delta\tau^{\mathrm{aod}} m_{\mathrm{aod}}$$

where

$$\Delta\tau^{\mathrm{R}} = \textstyle\sum_i W_i \tau_i^{\mathrm{R}} \;\; ; \;\; \Delta\alpha^{\mathrm{O_3}} = \textstyle\sum_i W_i \alpha_i^{\mathrm{O_3}}$$

$W_i(Dobsons) = (+1, -1, +1, -1)$ and $W_i(Brewers) = (+1, -0.5, -2.2, +1.7)$, with $\sum_i W_i = 0$.

$$\Delta\tau^{\mathrm{aod}} = \textstyle\sum_i W_i \tau_i^{\mathrm{aod}} \approx 0$$

$$F = F_0 - \Delta\tau^{\mathrm{R}} m_{\mathrm{R}} - \Delta\alpha^{\mathrm{O_3}} X m_{\mathrm{O_3}}$$

$$\boxed{TOC = X = \frac{F_0 - F - \Delta\tau^{\mathrm{R}} m_{\mathrm{R}}}{\Delta\alpha^{\mathrm{O_3}} m_{\mathrm{O_3}}}}$$

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Procedure of Simulation

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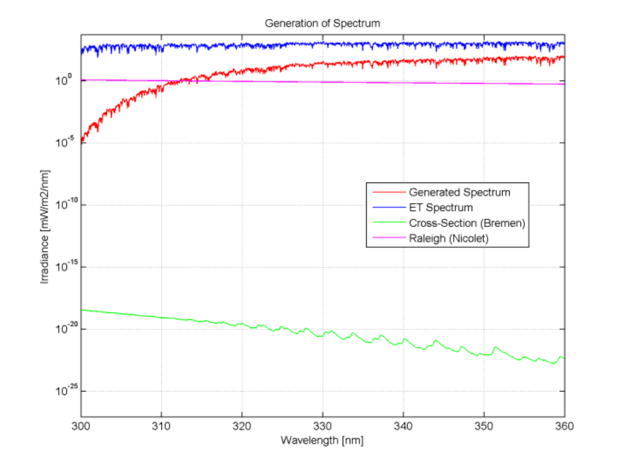

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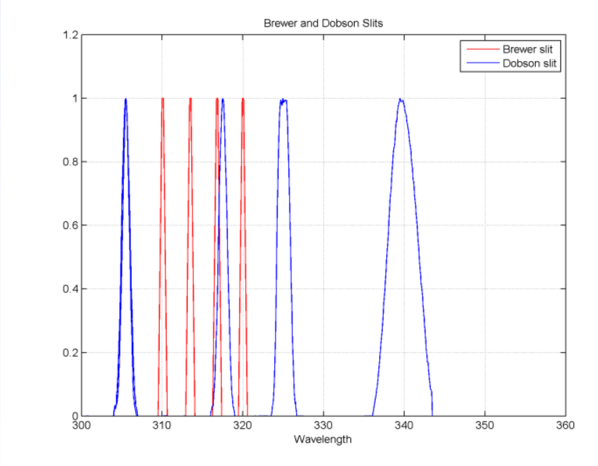
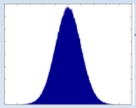
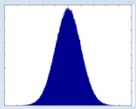
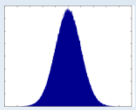
$$\boxed{TOC = X = \frac{F_0 - F - \Delta\tau^{\mathrm{R}} m_{\mathrm{R}}}{\Delta\alpha^{\mathrm{O_3}} m_{\mathrm{O_3}}}}$$

calculating **integral** over the slits



Procedure of Simulation

3. Random variation of uncertain parameters

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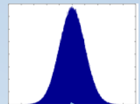
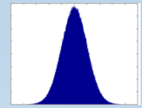
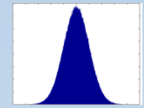

$$TOC = X = \frac{F_0 - F - \Delta\tau^{\mathrm{R}} m_{\mathrm{R}}}{\Delta\alpha^{\mathrm{O}_3} m_{\mathrm{O}_3}}$$

= Uncertainty of **O_3 value**

Uncertainty of **measurement:** +

- noise of the measurement
- wavelength uncertainty
- uncertainty of calibration
- bandpass uncertainty
- temperature gradients
- dead-time effect /linearity
- ND filter

Uncertainty of **model**:

- selected wavelengths (Brewer/Dobsons)
- selected cross-section
- selected atmospheric temperature
- extraterrestrial spectrum
- airmass uncertainty (atmospheric profile)
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= Uncertainty of **O_3 value**

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Procedure of Simulation

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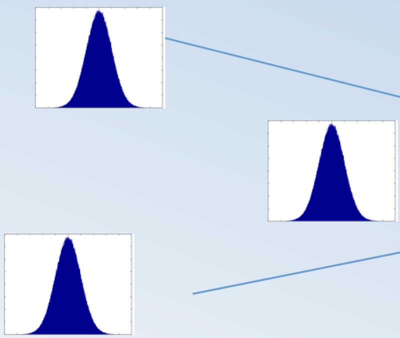
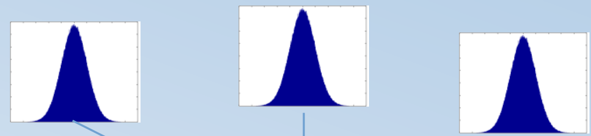




$$\boldsymbol{+} \quad TOC = X = \frac{F_0 - F - \Delta\tau^{\mathrm{R}} m_{\mathrm{R}}}{\Delta\alpha^{\mathrm{O_3}} m_{\mathrm{O_3}}} \quad \boldsymbol{=}$$

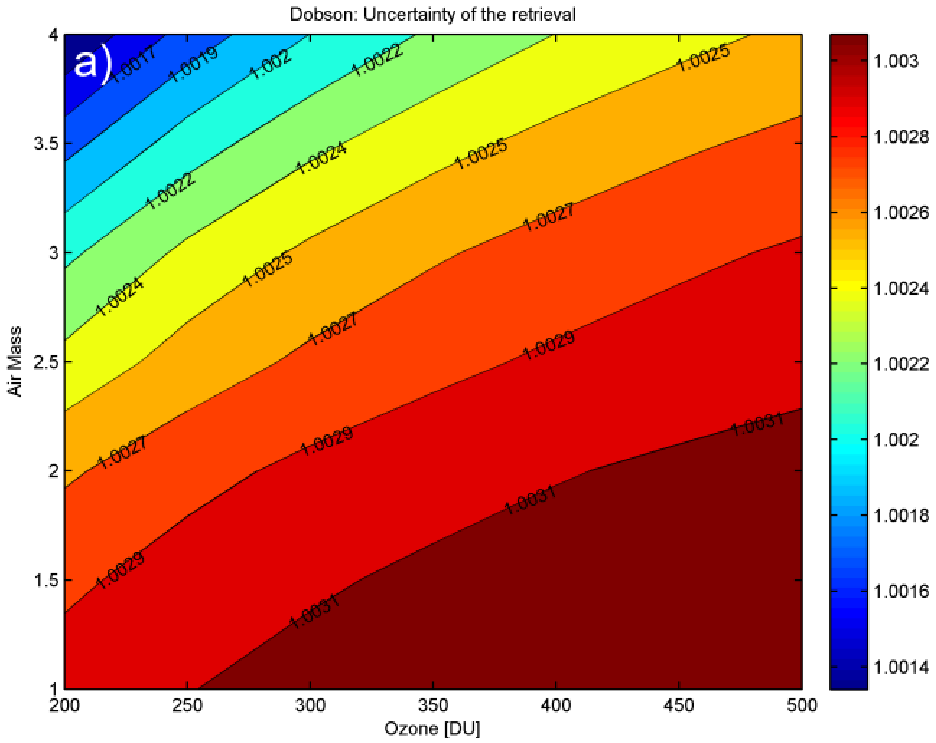
Uncertainty of **O_3 value**

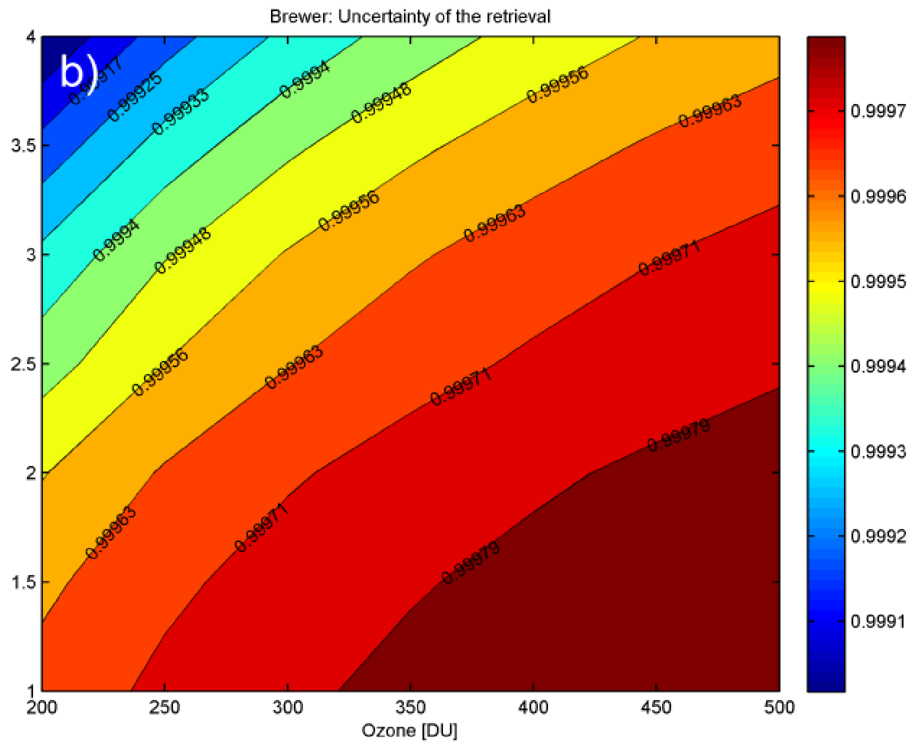
4. Making 100 runs with random variation, for all 49 atmospheric conditions

5. Comparison (ratio) between **input ozone** (no variation) and **retrieved ozone**

Uncertainty = standard deviation of all ratios

First Result: No Variation





Dobson: 0.14% -0.3 % (systematic)

Brewer: 0.02% - 0.1% (systematic)

Simulation works.

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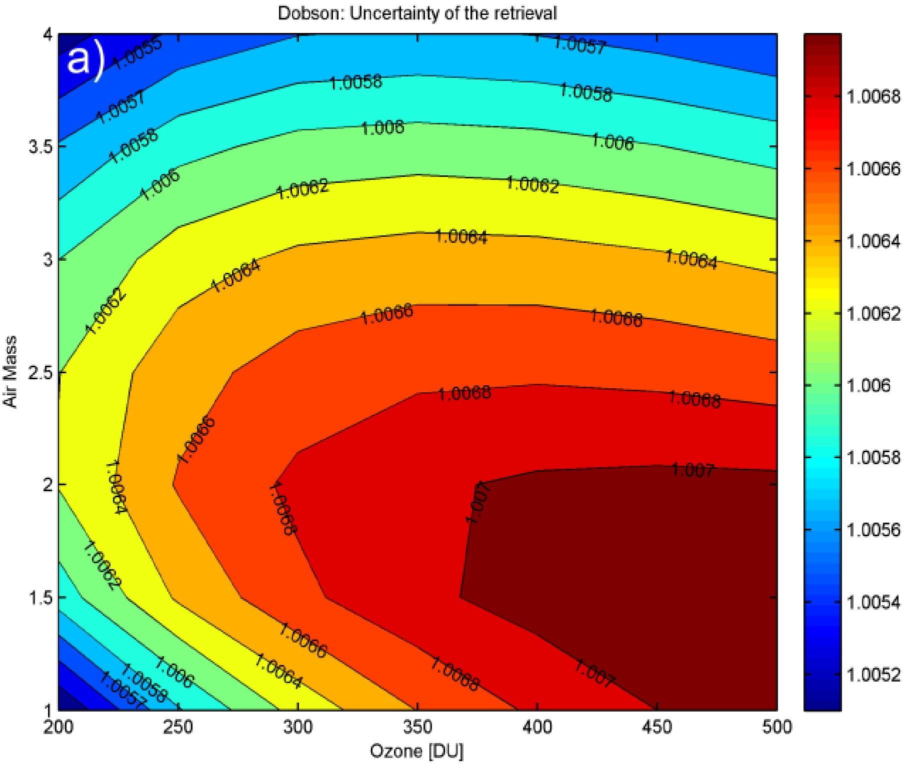
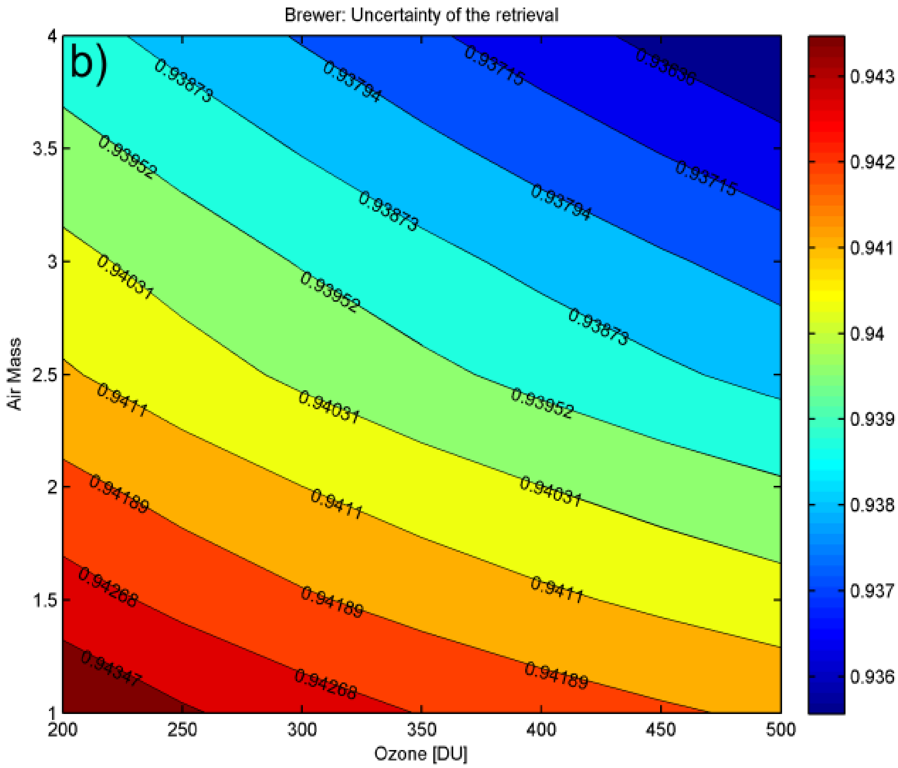
First Result: Array SRM

FWHM of generated spectrum: 0.5 nm (not 0.01nm), sampling resolution: 0.2 nm



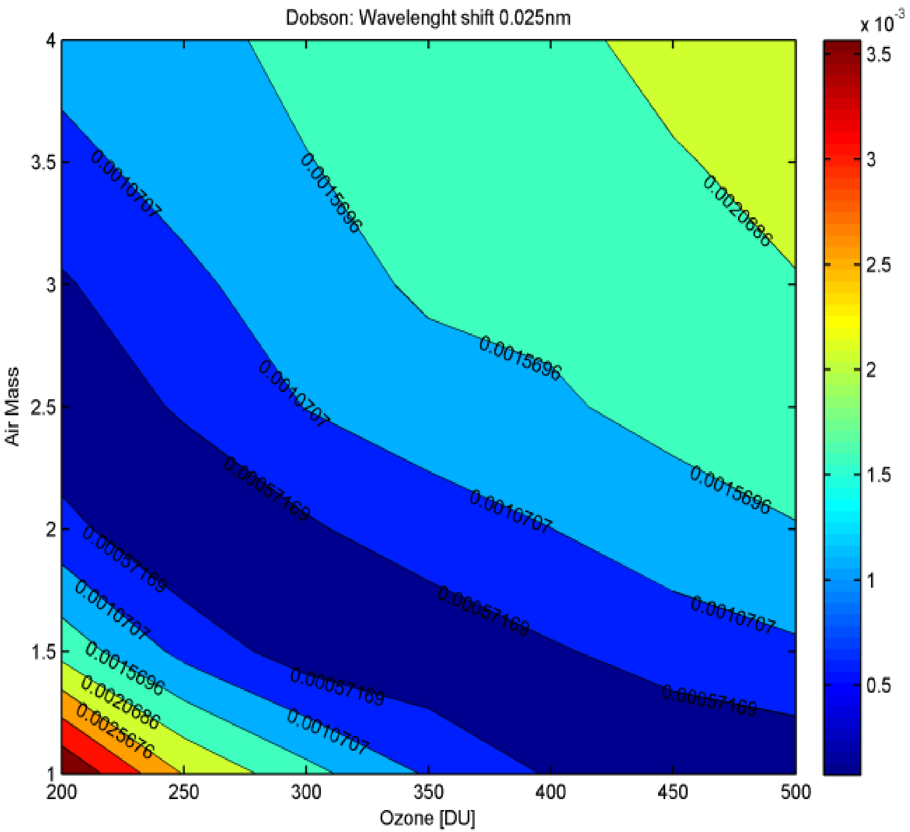


Dobson: 0.5% -0.7 % (systematic) **Brewer:** -6.4% - 5.6% (systematic)

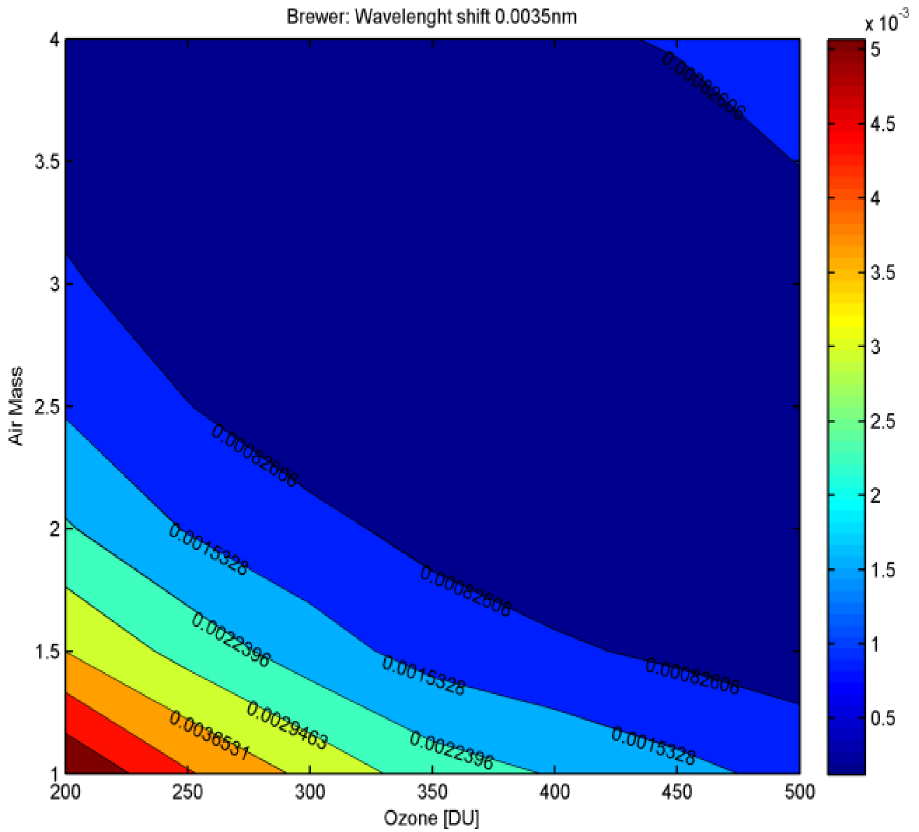
Retrieval **does not** work for spectra of array spectroradiometer.
Systematic bias can be eliminated by **Langley calibration**

Variation of wavelength shift

Variation of wavelength-shift of input spectrum: ±0.025 / (±0.0035) nm



Dobson: 0.05% - 0.35%



Brewer: 0.05% - 0.5%

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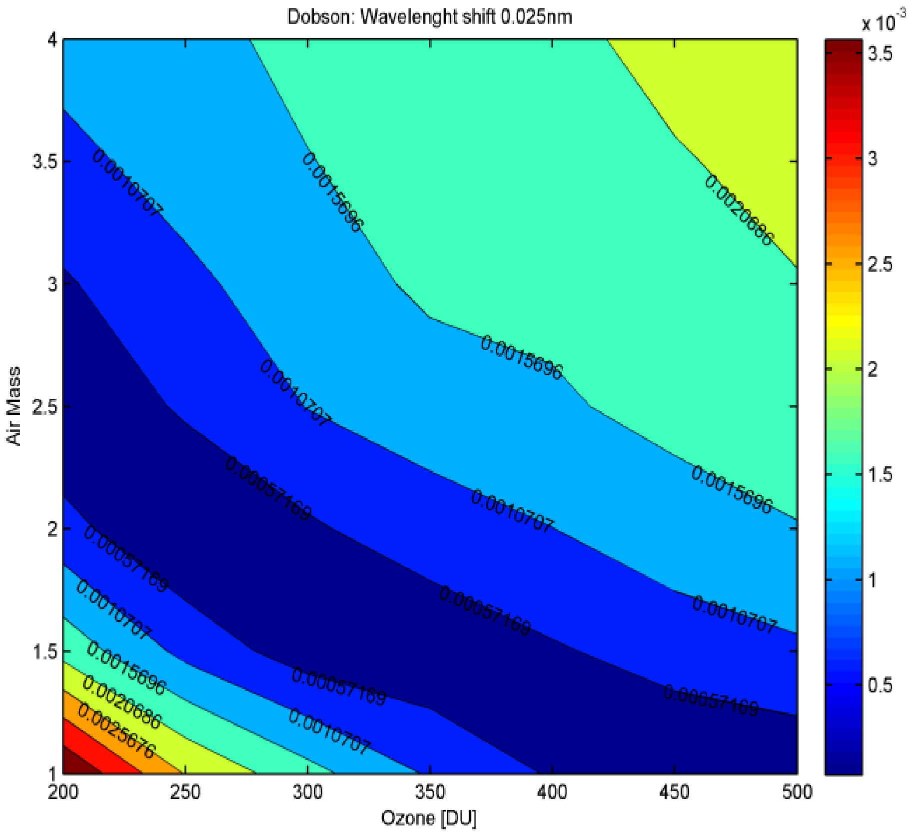
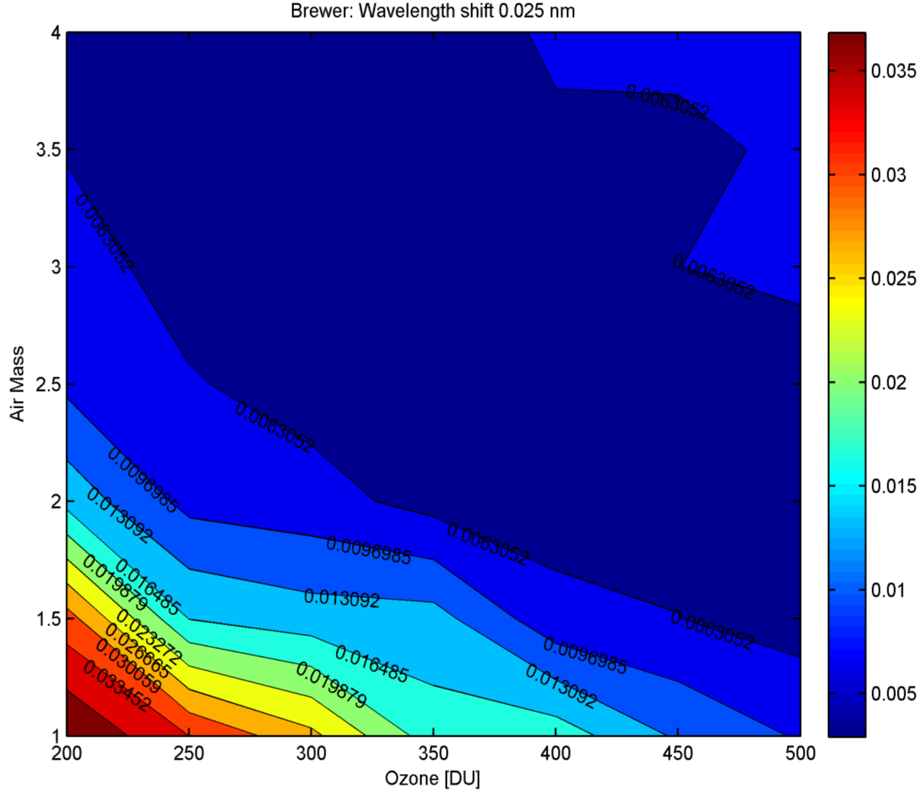
Variation of wavelength shift

Variation of wavelength-shift of input spectrum: ±0.025 / (±0.0035) nm





Dobson: 0.05% - 0.35%

Brewer: 0.5% - 3.5%

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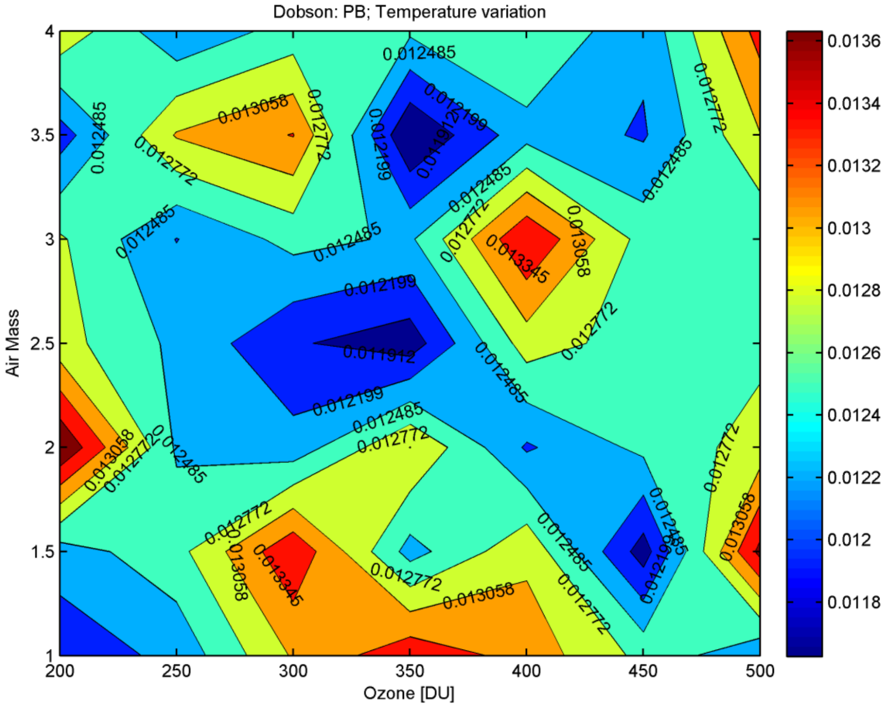
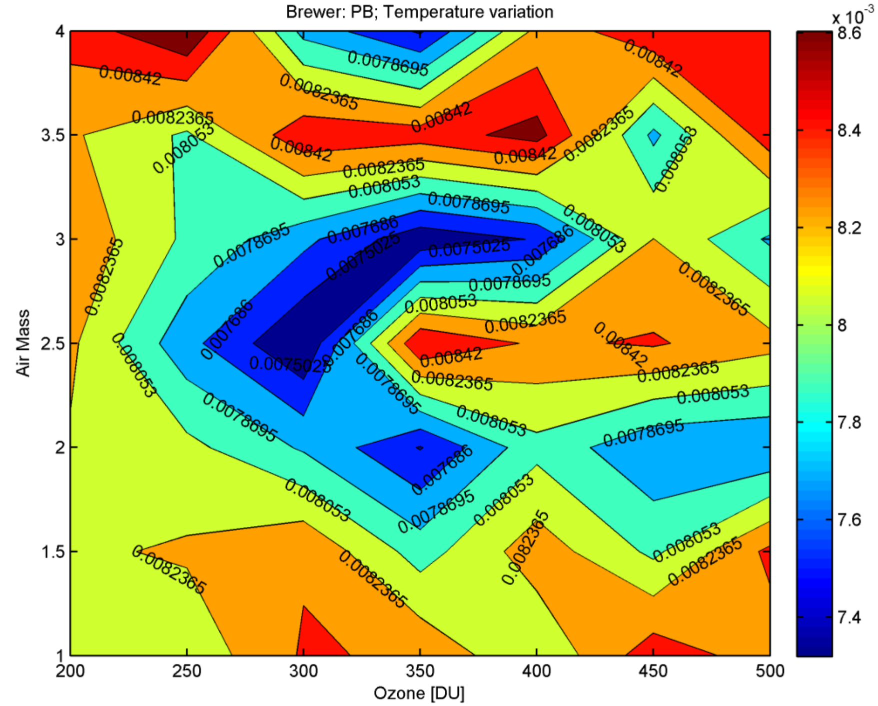
Result: Stratospheric Temperature

Variation of stratospheric temperature (retrieval): 213K – 243K: **«Bass-Paur»**





Dobson: 1.2% - 1.4%

Brewer: 0.7% - 0.9%

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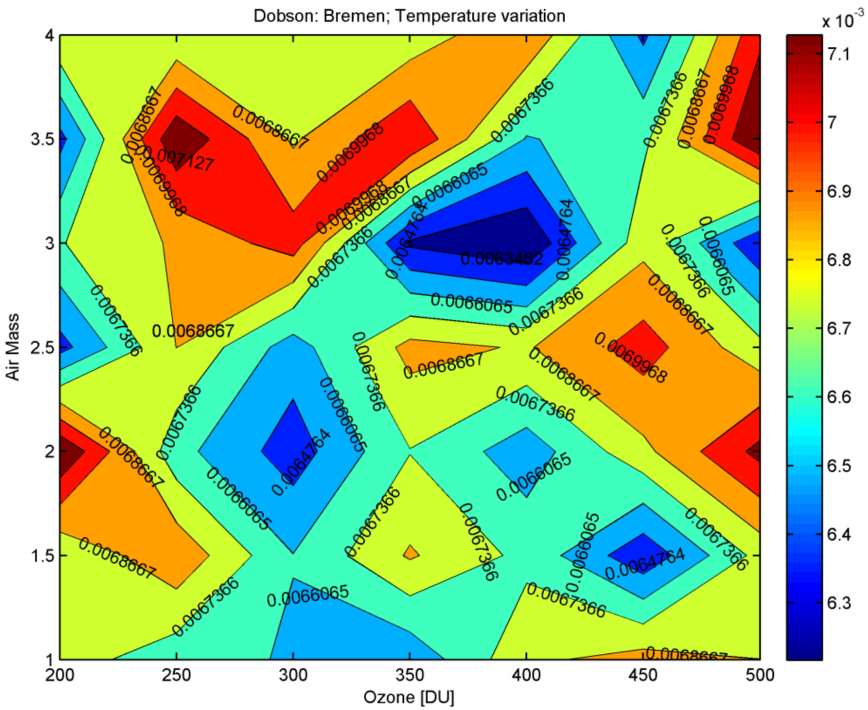
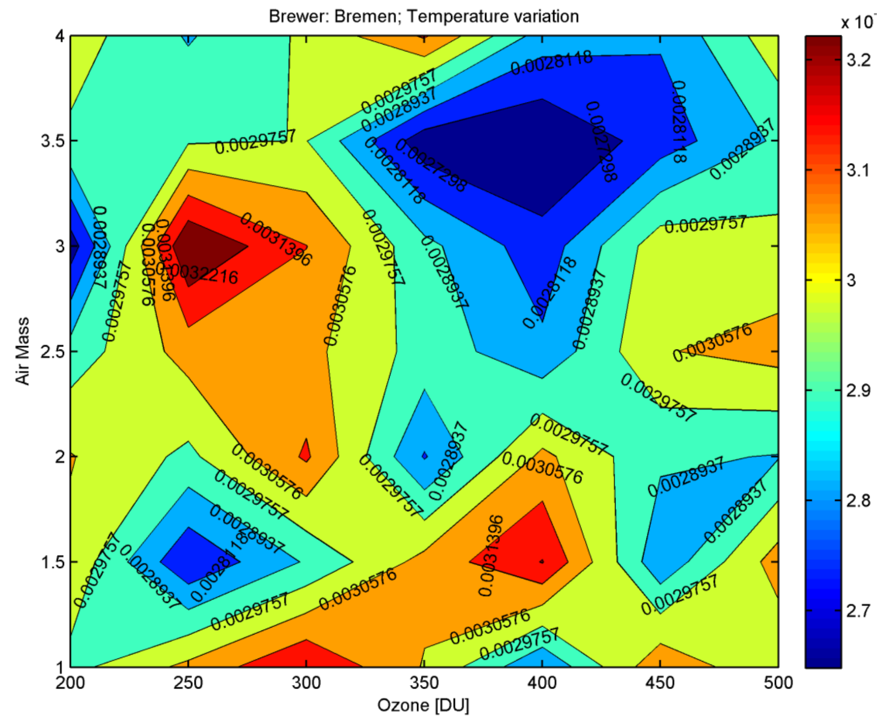
Result: Stratospheric Temperature

Variation of stratospheric temperature (retrieval): 213K – 243K: **«Bremen»**





Dobson: 0.6% - 0.7%

Brewer: 0.27% - 0.32%

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Summary Sensitivity

Averaged uncertainty of **Ozone** over all atmospheric conditions:

	Dobsons	Brewer	**Remark**
Wavelength ±0.025 nm	0.1%	0.9%	
Noise of detector /Calibration /ND filter Deadtime /linearity/ Instr. Temperature ±0.1%	0.06%	0.4%	linear
Strat. Temp Bass-Paur: 213K-243 K	1.2%	0.8%	
Strat. Temp Bremen: 213K-243 K	0.6%	0.3%	
Cross-Section Bass-Paur: ±5%	1.2%	2.4%	
Extraterrestrial : ±5%	0%	0%	Uncertainty from Langley?
Ozone Air Mass Variation	linear	linear	Uncertainty of air mass need to be investigated
AOD / SO2	?	?	Need to be investigated

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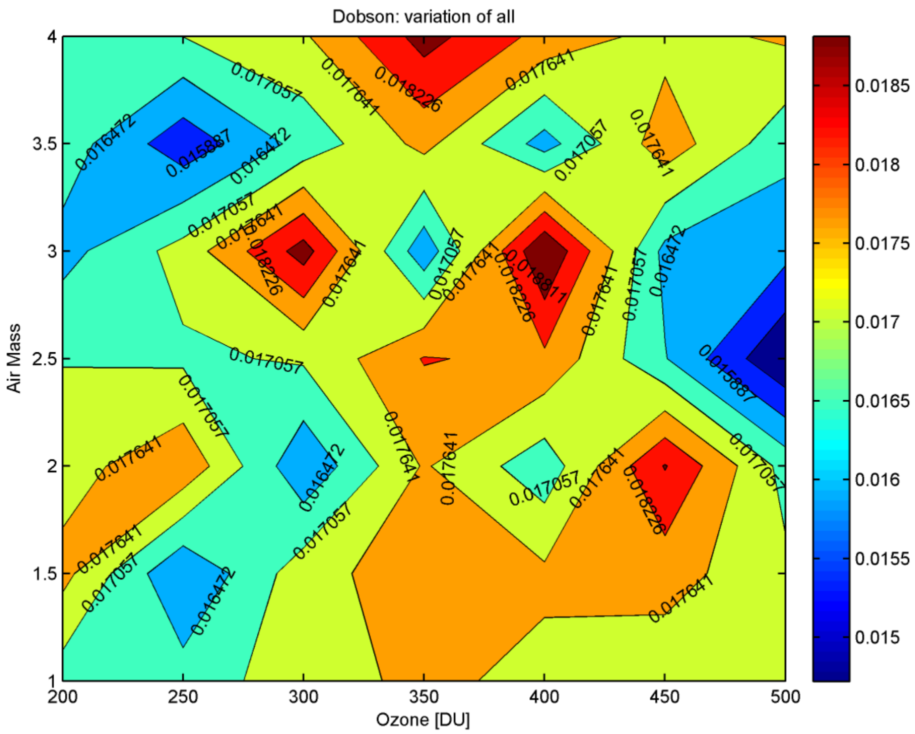
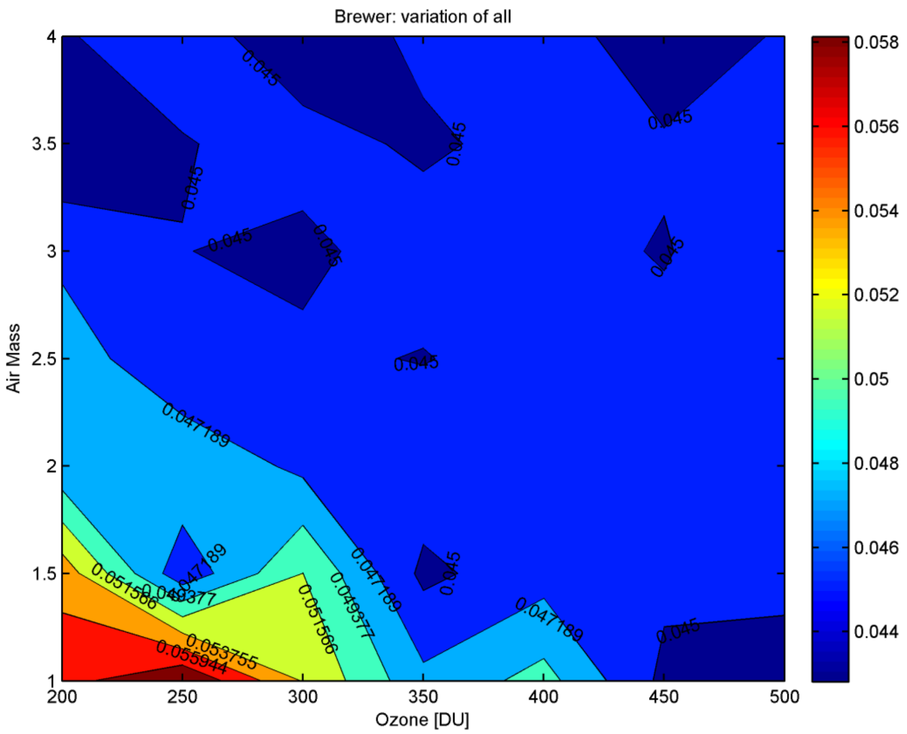
Variation of all Parameters

Variation of uncertain input and model parameters:

Wavelength ±0.025 nm; Calib: ±0.1%; Bass-Paur, Temp. 213-243K, Variation of cross section ±5%





Dobson: 1.5% - 1.9% = **1.7%**

Brewer: 4.4% - 5.8% = **4.6%**

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Summary Sensitivity

«Uncertainty reduction» by convention (identical cross-sections, ET etc.)

	Dobsons	Brewer	**Remark**
Wavelength ±0.025 nm	0.1%	0.9%	
Noise of detector /Calibration /ND filter Deadtime /linearity/ Instr. Temperature ±0.1%	0.06%	0.4%	linear
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Ozone Air Mass Variation	linear	linear	Uncertainty of air mass need to be investigated
AOD / SO2	?	?	Need to be investigated

«Harmonized instrument network»

Summary Sensitivity

«Uncertainty reduction» by convention (identical cross-sections, ET etc.)

Discussion / Decision

SAG Ozone

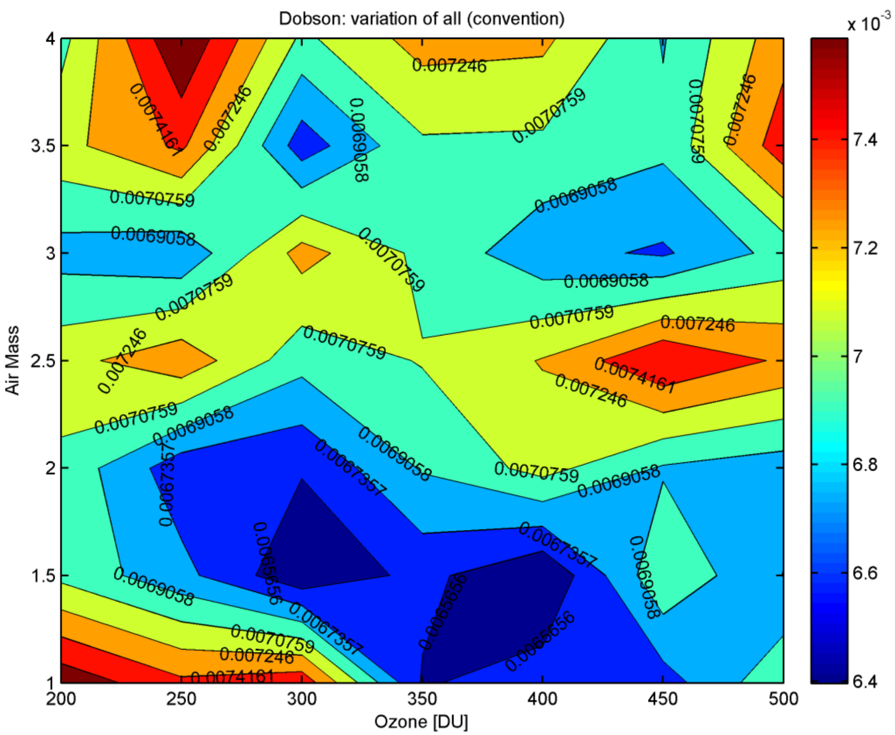
Scientific Steering Commitee ATMOZ

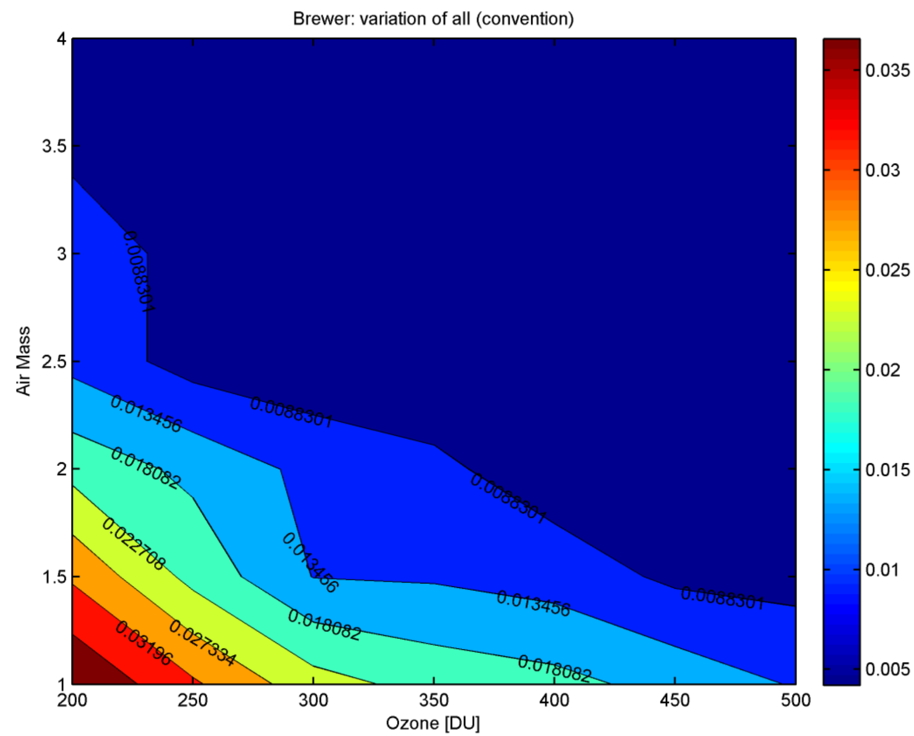
Bass-Paur: 213K-243 K			
Strat. Temp Bremen: 213K-243 K	0.6%	0.3%	
Cross-Section Bass-Paur: ±5%	1.2%	2.4%	
Extraterrestrial : ±5%	0%	0%	Uncertainty from Langley?
Ozone Air Mass Variation	linear	linear	Uncertainty of air mass need to be investigated
AOD / SO2	?	?	Need to be investigated

«Harmonized instrument network»

Variation of all Parameters

Variation of **parameters,** which cannot be determined by convention
Wavelength ±0.025 nm; Calib: ±0.1%; Bremen, Temp. 213-243K





Dobson: 0.6% - 0.75% **= 0.7%**

Brewer: 0.5% - 3.5% **=1.1%**

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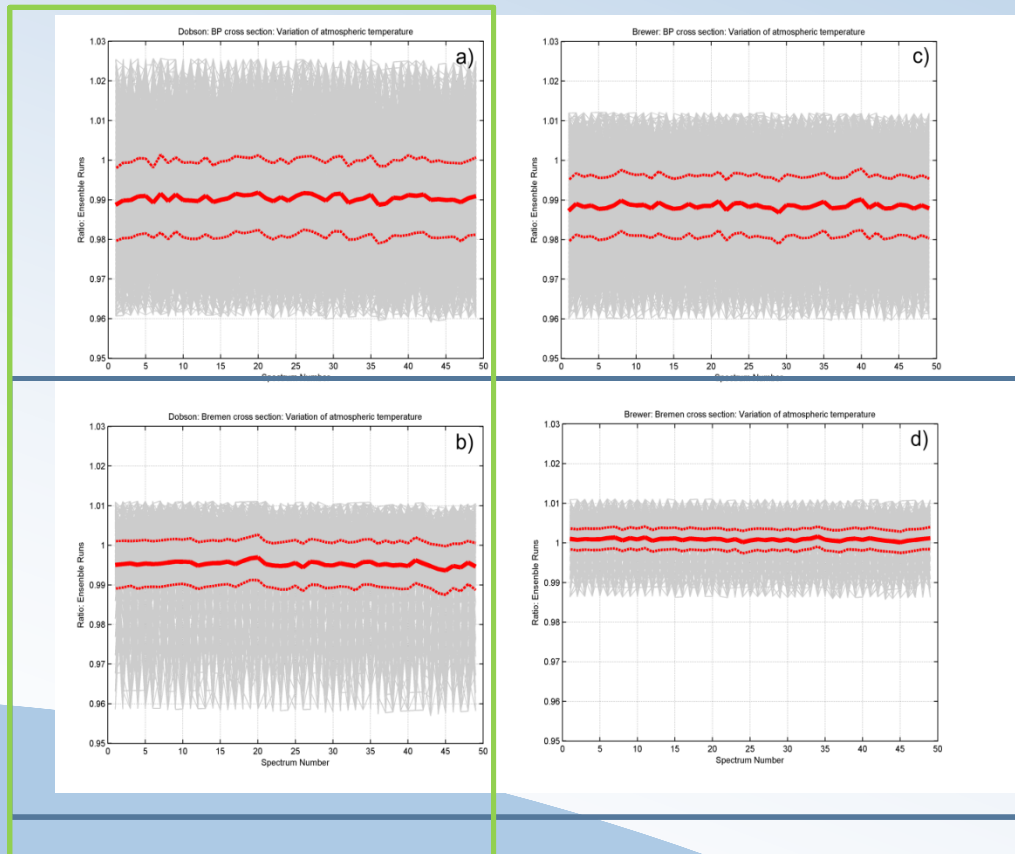
Conclusions

- **Dobson** show generally a **lower uncertainty budget** than **Brewers**
- Reducing **wavelength and calibration uncertainty** is crucial for Brewers
- **Brewers** show a **less sensitivity to stratospheric temperature** variation than Dobsons
- **“Bremen” cross section is less sensitive** to stratospheric temperature variations



«Bremen»

Dobson

Conclusions

- Uncertainties of **signal at each individual slit** is essential and may be composed of:
  - Calibration
  - Intensity of sun (airmass)
  - ND filters
  - Dead time / linearity
  - Temperature gradients of instruments

The impact of these effects on the **uncertainty of the signal** should be investigated individually to obtain **one general uncertainty of signal.**

pmod wrc

Outlook

- Uncertainty of **Langley plot calibration** need to be quantified
- Stratospheric **temperature should be known** to reduce uncertainty
- Working on **method to retrieve stratospheric temperature** from direct sun measurements
- The software will be used to **determine the overall uncertainty** from Dobson / Brewer and array spectroradiometer measurements

Array SRM	NEI=**0.1mW**	NEI=**0.01mW**	**Remark**
Wavelength ±0.05 nm	1% (Full Spec.) 1.5% (Multi Double Ratio)	0.6% (Full Spec.) 1.1% (Multi Double Ratio)	Depending on FWHM
Calibration ±5%	1.1% 2%	0.7% 1.4%	Constant factor: No effect
Extraterrestrial ±2%	0.6% 0.7%	0.2% 0.3%	Constant factor: No effect
Strat. Temp Bremen: 213K-243 K	0.9% 1.1%	0.7% 0.8%	Bremen Recommended
Cross-Section Var. Bremen: ±5%	0.8% 0.6%	0.4% 0.1%	Depending on FWHM

wrc

Outlook

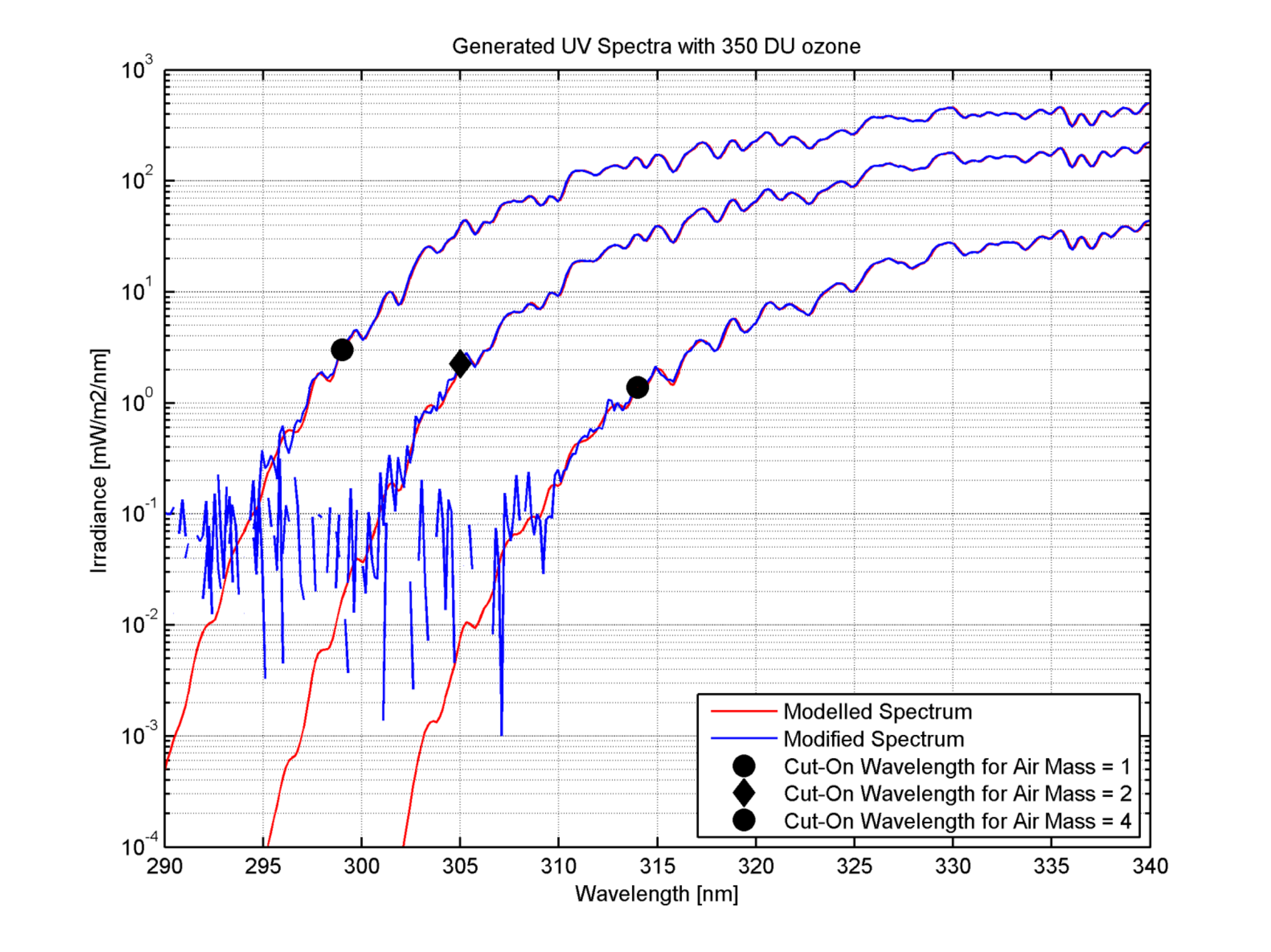
- Uncertainty of **Langley plot calibration** need to be quantified
- Stratospheric **temperature should be known** to reduce uncertainty
- Working on **method to retrieve stratospheric temperature** from direct sun measurements
- The software will be used to **determine the overall uncertainty** from <u>Dobson / Brewer</u> and <u>array spectroradiometer measurements</u>, in combination with **other approaches.**

Array SRM	NEI=**0.1mW**	NEI=**0.01mW**	Remark
Wavelength ±0.05 nm	1% (Full Spec.) 1.5% (Multi Double Ratio)	0.6% (Ful 1.1% (Multi	
Calibration ±5%	1.1% 2%	0.7% 1.4%	Constant factor: No effect
Extraterrestrial ±2%	0.6% 0.7%	0.2% 0.3%	Constant factor: No effect
Strat. Temp Bremen: 213K-243 K	0.9% 1.1%	0.7% 0.8%	Bremen Recommended
Cross-Section Var. Bremen: ±5%	0.8% 0.6%	0.4% 0.1%	Depending on FWHM

Next Talk: Petri Kärhä

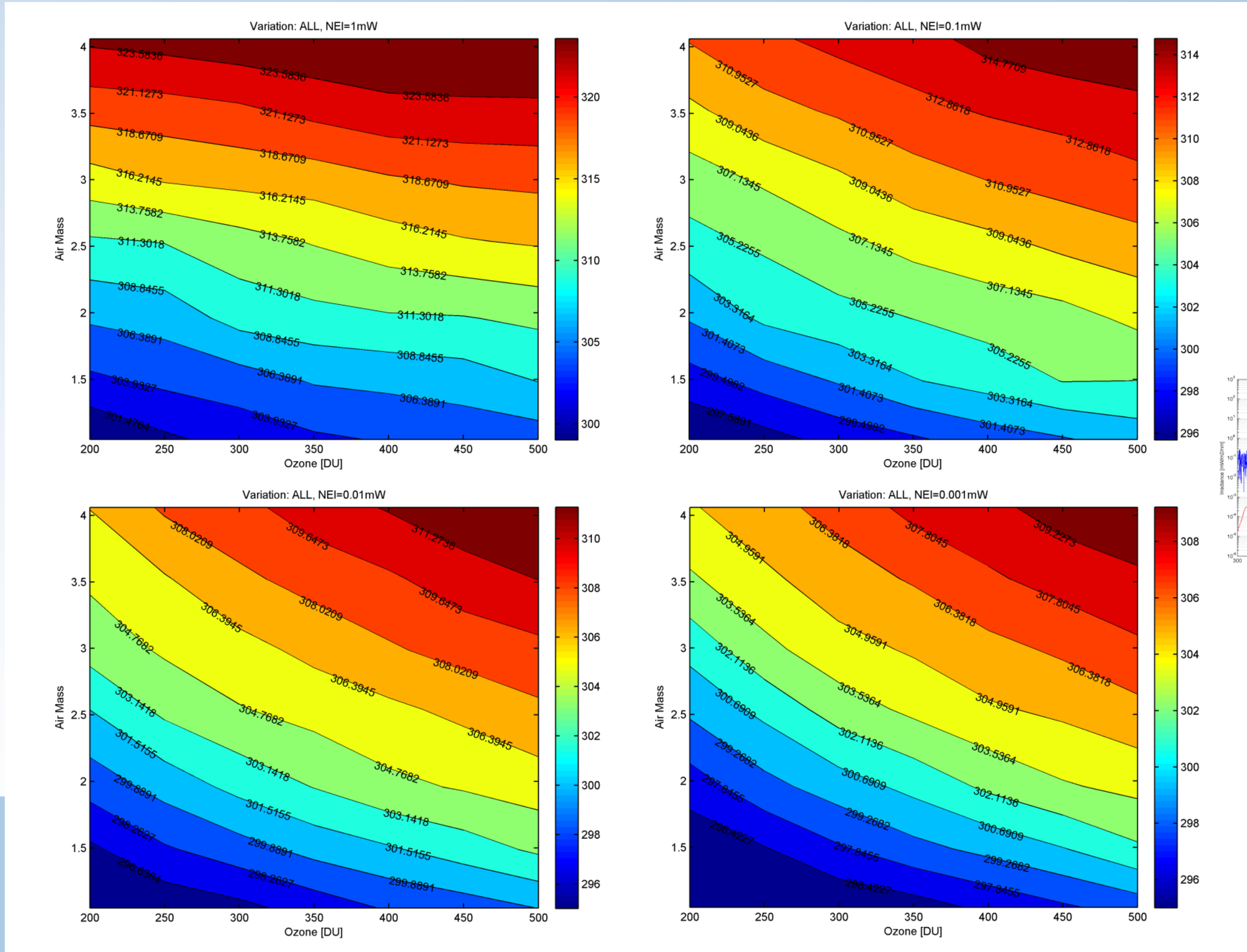
Array Spectroradiometer (full spectrum)

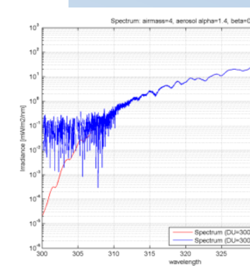
Automatic detection of cut-on wavelength



pmod wrc

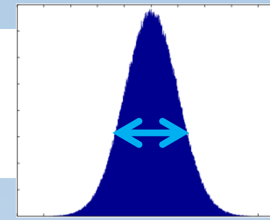
Cut-On Wavelength

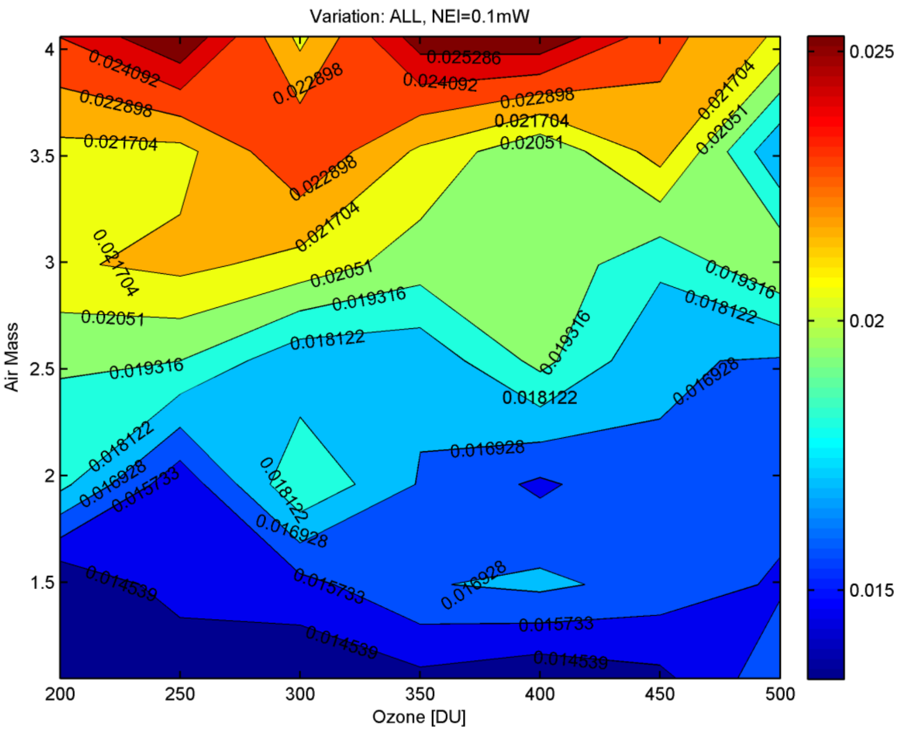


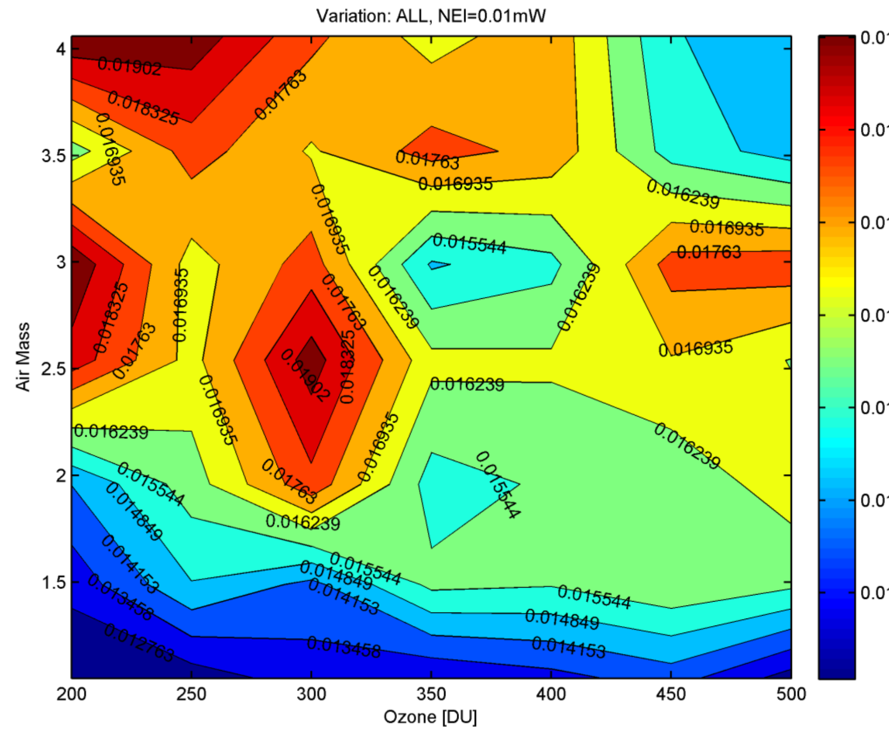


Variation of all Parameters

Variation of **all uncertain input** and **model parameters** (500 runs):
Bass-Paur crosssection / consistent networks







NEI=0.1mW: **1.5% - 2.5%** / **0.8%-2.2%**

NEI=0.01mW: 1.8% - 3.8% (Double ratio)

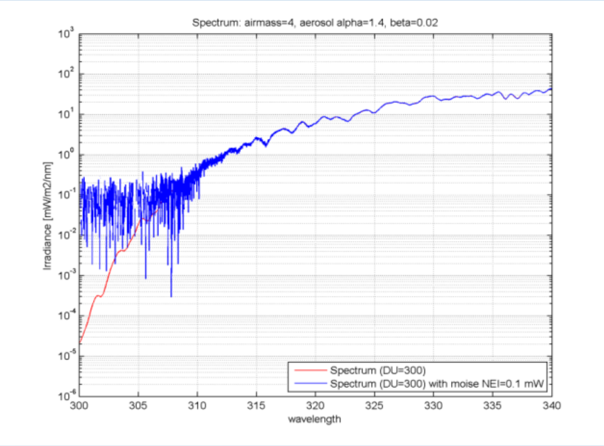
NEI=0.01mW: **1.3% - 1.9%** / **0.7%-1.3%**

NEI=0.01mW: 1.6% - 3% (Double ratio)

Conclusions

Overall uncertainty of ozone retrieval by multispectral measurements depends mainly on

- **NEI = Noise equivalent Irradiance** => impact on selection of usable wavelength range
- Wavelength uncertainty
- Atmospheric conditions (mainly air-mass)
- Air-mass determination



Less contributions for the overall uncertainty are from:

- Selected X-sections; Variations of X-section **-> convention to select one specific X-section** (recommendation: "Bremen X-section -> new generation in ATMOZ)
- Variation of extraterrestrial spectrum **-> convention to select one specific ET** (new measurements and validation in ATMOZ)
- Random Variation of input spectrum
- Stratospheric Temperature **-> retrieving stratospheric temperature** (on-going research)
- Bandpass (except in combination with wavelength shift)
- Resolution (small impact on random variation)

pmod wrc

Conclusions

Overall uncertainty of ozone retrieval by multispectral measurements depends mainly on

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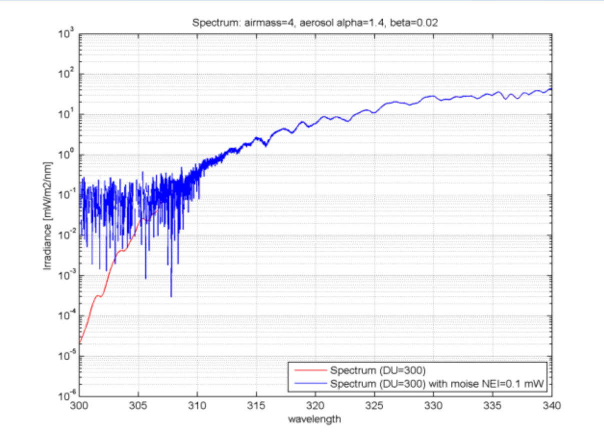

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